Design of High Thermal Conductivity Polymers based on a Bayesian machine learning approach

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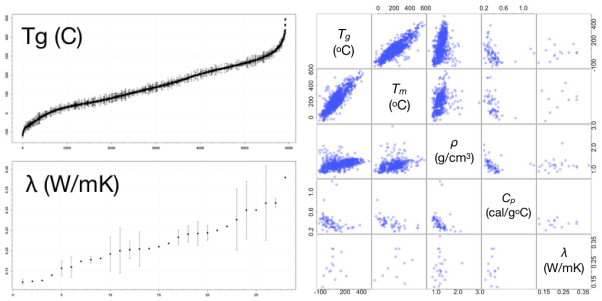
Data

PolyInfo

Glass transition temperature (Tg)
Melting temperature (Tm)
Density (ρ)
Heat capacity at constant pressure (Cp)
Thermal conductivity (λ)

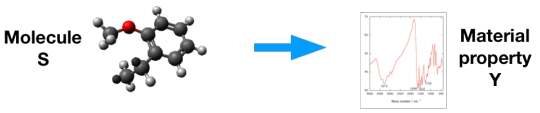
QM9 database

Heat capacity at constant volume (Cv)



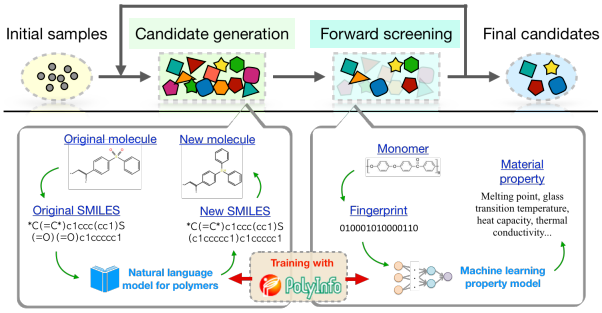
Algorithm

Forward prediction



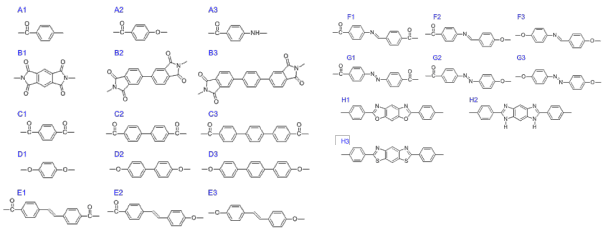
Bayesian inverse design

$$p(S|Y) \propto p(Y|S)p(S)$$



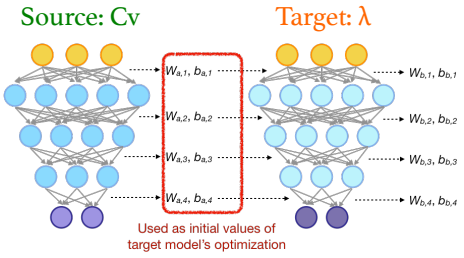
Screening 1

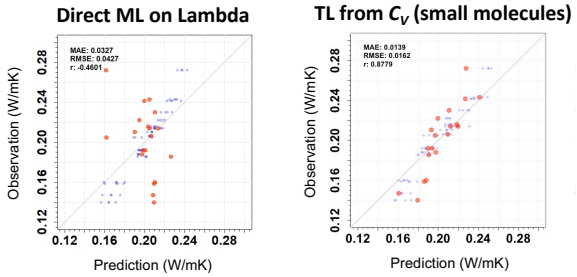
Expert knowledge on processability in practice:
Consider candidates that include
a given list of substructures



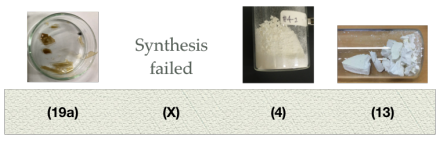
Screening 2

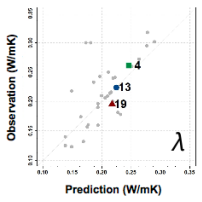
λ model with transfer learning





Results





Polymer	4 (pre)	4 (obs)	4 (anneal)	13(pre)	13 (obs)	13 (anneal)	19 (pre)	19a (obs)
T_g (°C) (DSC)	286	N/A*	-	228	N/A*	-	121	194
T_g (°C) (FSC)	286	221	-	228	226	-	121	191
T_m (°C) (FSC)	404	513	-	426	494	-	321	303
α (mm^2/s)	-	0.168	0.263	-	0.152	0.254	-	0.133
C_P (at 25–27°C)	-	1.13	-	-	1.14	1.10	-	1.19
ρ (at 16–20°C)	1.308	1.373	-	1.288	1.295	1.386	1.260	1.233
λ (W/mK)	0.246	0.261	0.408**	0.225	0.224	0.387	0.218	0.195
η_{inh} (dL/g)	-	0.193	-	-	0.317	-	-	0.313
TG_{10} (°C)	-	400	-	-	>500	-	-	361
Xc	-	0.16	-	-	0.30	0.30	-	0.09#

On-going

All-in-one materials design Python package: XenonPy

Github

Readme